LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	500	504	517	rVB	185127	216833	14.16%	1.204%
2	5.469	571	575	591	rBV	1131373	1179388	77.01%	6.548%
3	6.486	744	748	767	rBV	1209483	1265283	82.61%	7.025%
4	6.622	767	771	778	rVV	1685416	1363926	89.06%	7.573%
5	6.686	779	782	786	rVB	21271	24345	1.59%	0.135%
6	6.851	807	810	817	rBV	967757	804218	52.51%	4.465%
7	7.010	833	837	845	rBV	1228604	1097188	71.64%	6.092%
8	7.116	852	855	863	rVB	16353	18075	1.18%	0.100%
9	7.416	902	906	920	rBV	778018	745007	48.64%	4.136%
10	7.716	954	957	964	rVB	26394	30424	1.99%	0.169%
11	8.139	1025	1029	1046	rBV	1118757	1019094	66.54%	5.658%
12	8.357	1063	1066	1073	rBV	32733	32096	2.10%	0.178%
13	8.416	1073	1076	1085	rVB	34859	39004	2.55%	0.217%
14	8.851	1146	1150	1154	rBV2	20197	22136	1.45%	0.123%
15	9.216	1208	1212	1223	rBV	1811104	1531543	100.00%	8.503%
16	9.616	1277	1280	1286	rBV	122272	122563	8.00%	0.680%
17	9.898	1325	1328	1333	rBV	1129426	1026797	67.04%	5.701%
18	10.692	1460	1463	1478	rVB	795343	785737	51.30%	4.363%
19	11.392	1579	1582	1585	rBV	953712	925509	60.43%	5.139%
20	11.416	1585	1586	1593	rVV	181154	164170	10.72%	0.911%
21	11.474	1593	1596	1599	rVB	27847	25540	1.67%	0.142%
22	11.633	1617	1623	1627	rBV2	11720	20505	1.34%	0.114%
23	11.916	1663	1671	1679	rBV3	119557	205868	13.44%	1.143%
24	12.015	1684	1688	1690	rBV2	36699	41970	2.74%	0.233%
25	12.198	1715	1719	1722	rBV	20252	21354	1.39%	0.119%
26	12.233	1722	1725	1728	rVB	22925	27532	1.80%	0.153%
27	12.451	1759	1762	1764	rBV	25956	24322	1.59%	0.135%
28	12.545	1774	1778	1782	rBV2	22262	29457	1.92%	0.164%
29	12.615	1786	1790	1795	rBV	371301	349040	22.79%	1.938%
30	12.704	1803	1805	1810	rBV5	32988	40698	2.66%	0.226%
31	12.845	1823	1829	1836	rBV	347537	371678	24.27%	2.064%
32	12.898	1836	1838	1841	rVB2	23178	20949	1.37%	0.116%
33	12.980	1846	1852	1856	rBV	1508321	1420373	92.74%	7.886%
34	13.010	1856	1857	1862	rVB4	20436	19673	1.28%	0.109%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.062	1862	1866	1871	rBV3	23584	48592	3.17%	0.270%
36	13.157	1878	1882	1883	rBV4	33552	40513	2.65%	0.225%
37	13.174	1883	1885	1888	rVB2	37890	36748	2.40%	0.204%
38	13.239	1894	1896	1899	rVB2	25664	18648	1.22%	0.104%
39	13.280	1900	1903	1909	rVV3	35612	48356	3.16%	0.268%
40	13.374	1916	1919	1921	rBV	22431	27785	1.81%	0.154%
41	13.692	1971	1973	1977	rBV	29755	31253	2.04%	0.174%
42	13.874	2001	2004	2012	rVB3	165952	244418	15.96%	1.357%
43	14.051	2029	2034	2037	rBV2	1114029	1189216	77.65%	6.603%
44	14.074	2037	2038	2041	rVB	164854	94664	6.18%	0.526%
45	15.104	2210	2213	2217	rBV	134531	182049	11.89%	1.011%
46	15.156	2220	2222	2225	rVB	88848	75151	4.91%	0.417%
47	15.474	2274	2276	2282	rVB	92854	111264	7.26%	0.618%
48	15.545	2283	2288	2292	rBV	629597	830081	54.20%	4.609%

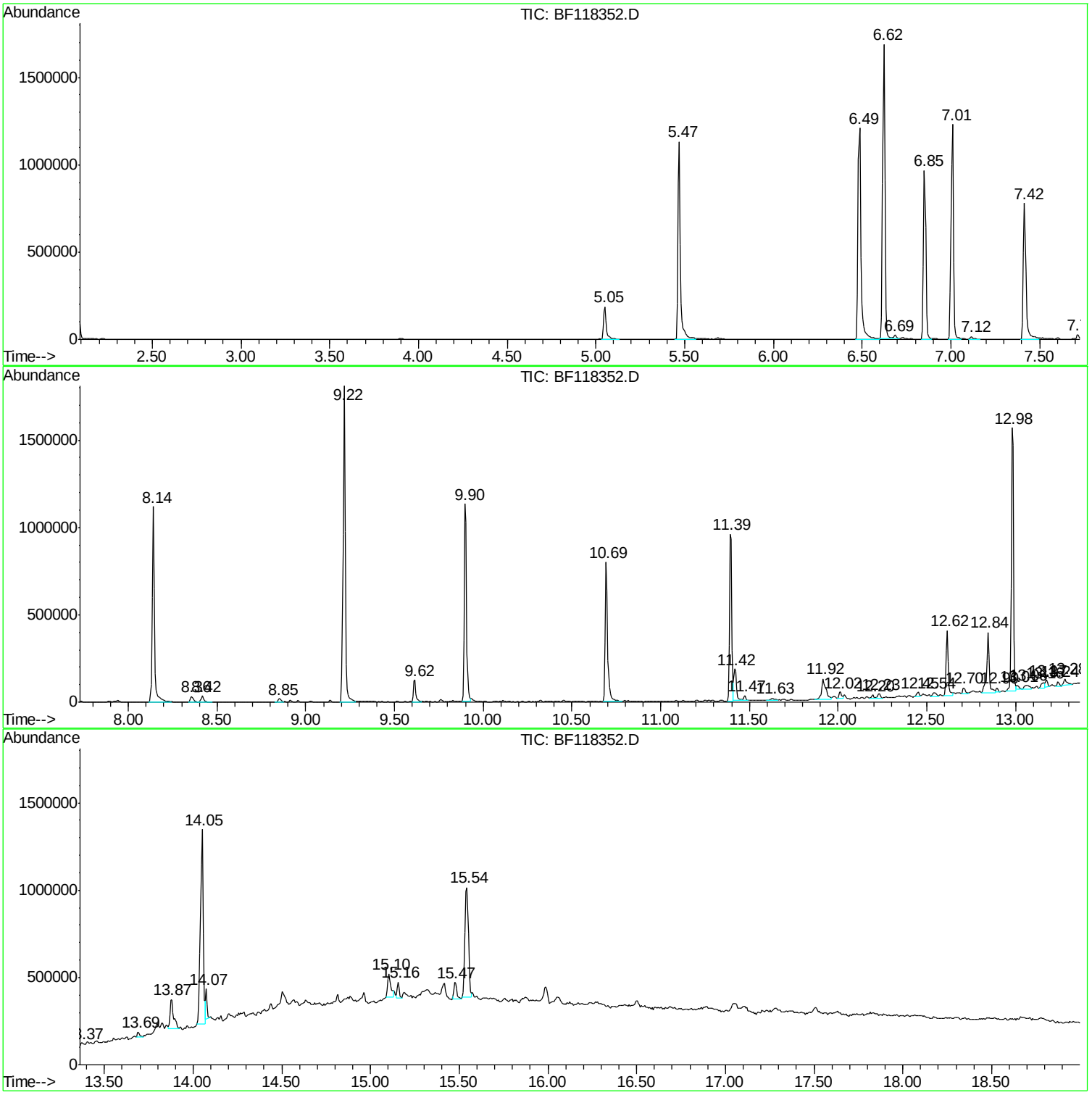
Sum of corrected areas: 18011033

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

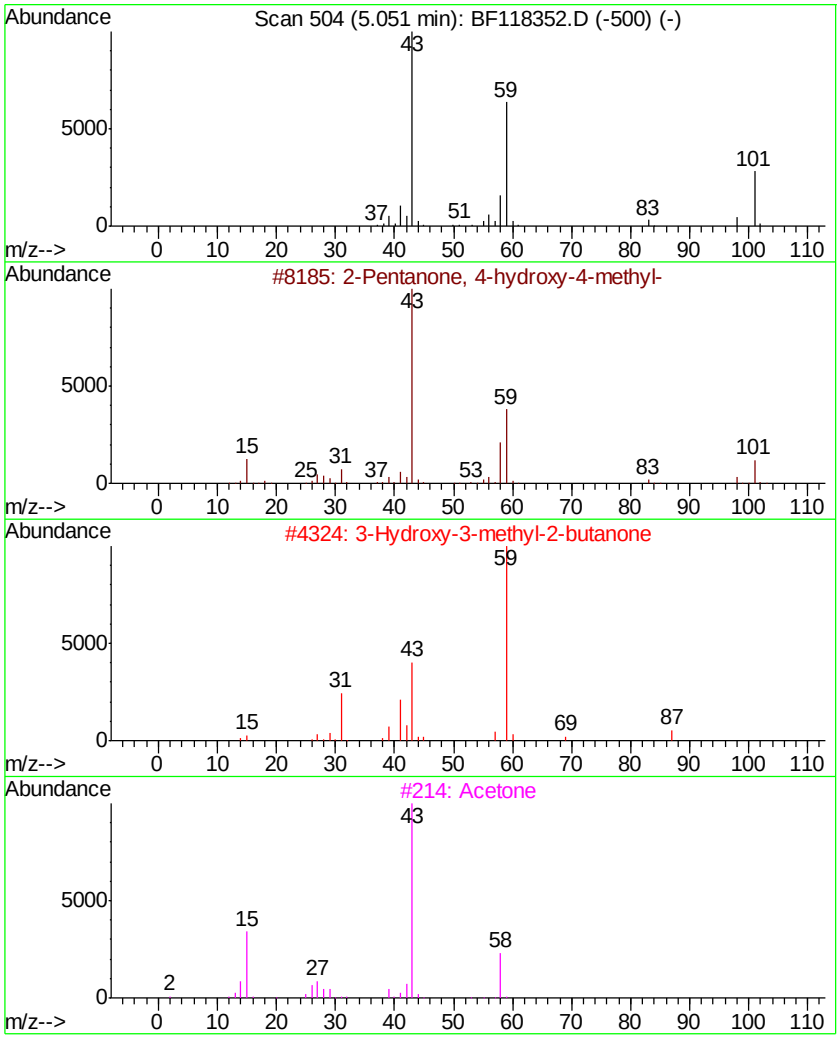
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

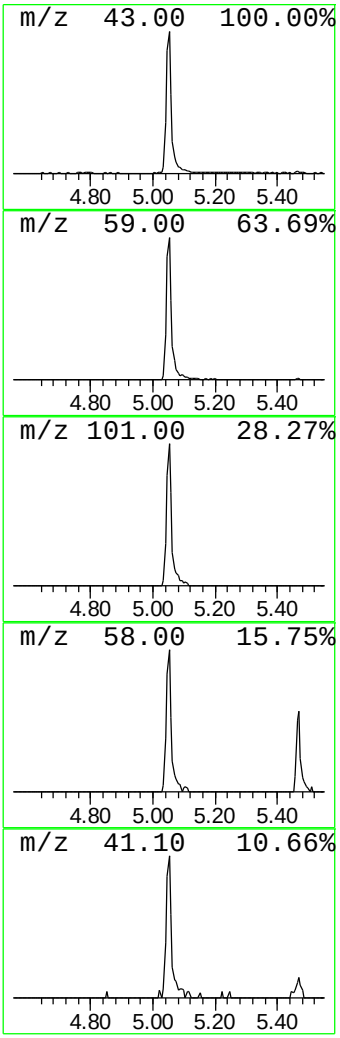
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	5.39 ng	216833	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	Acetone	58	C3H6O	000067-64-1	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

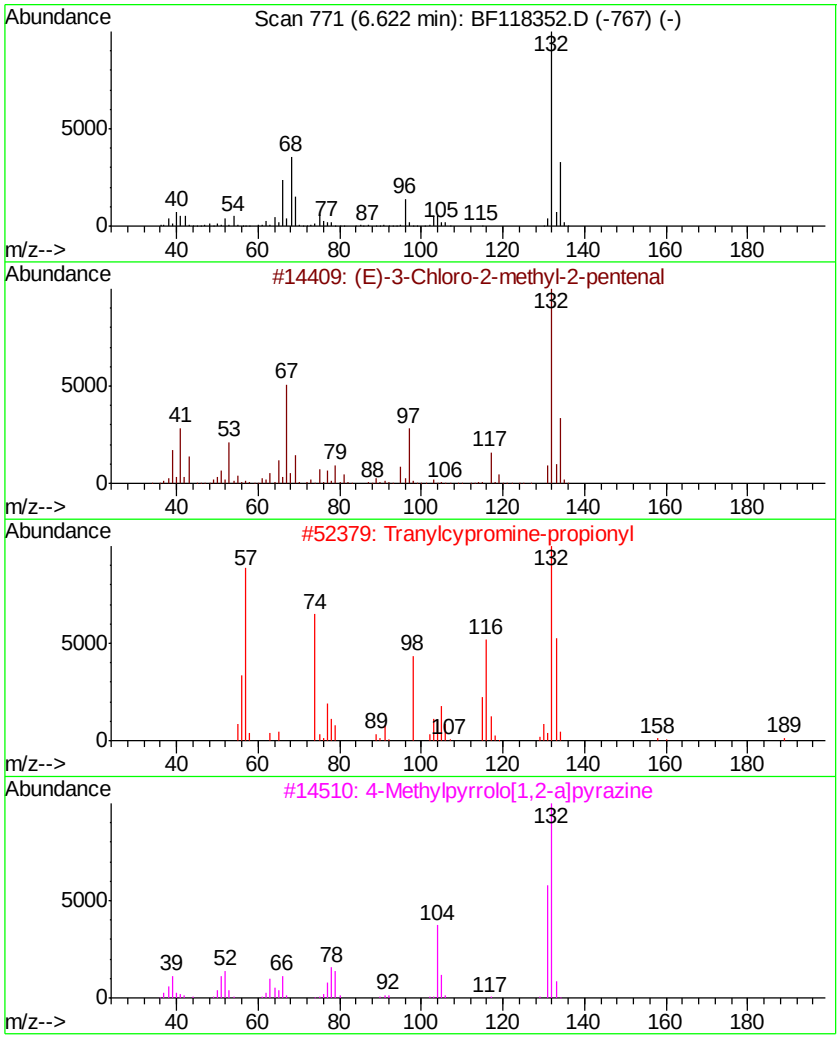
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

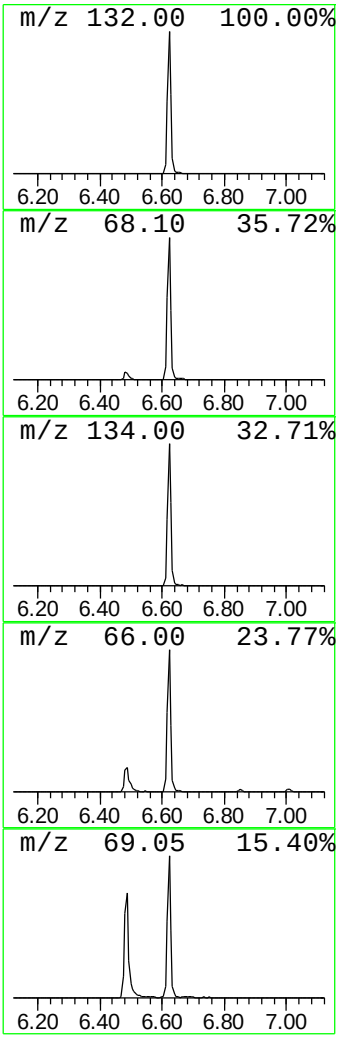
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	33.92 ng	1363930	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

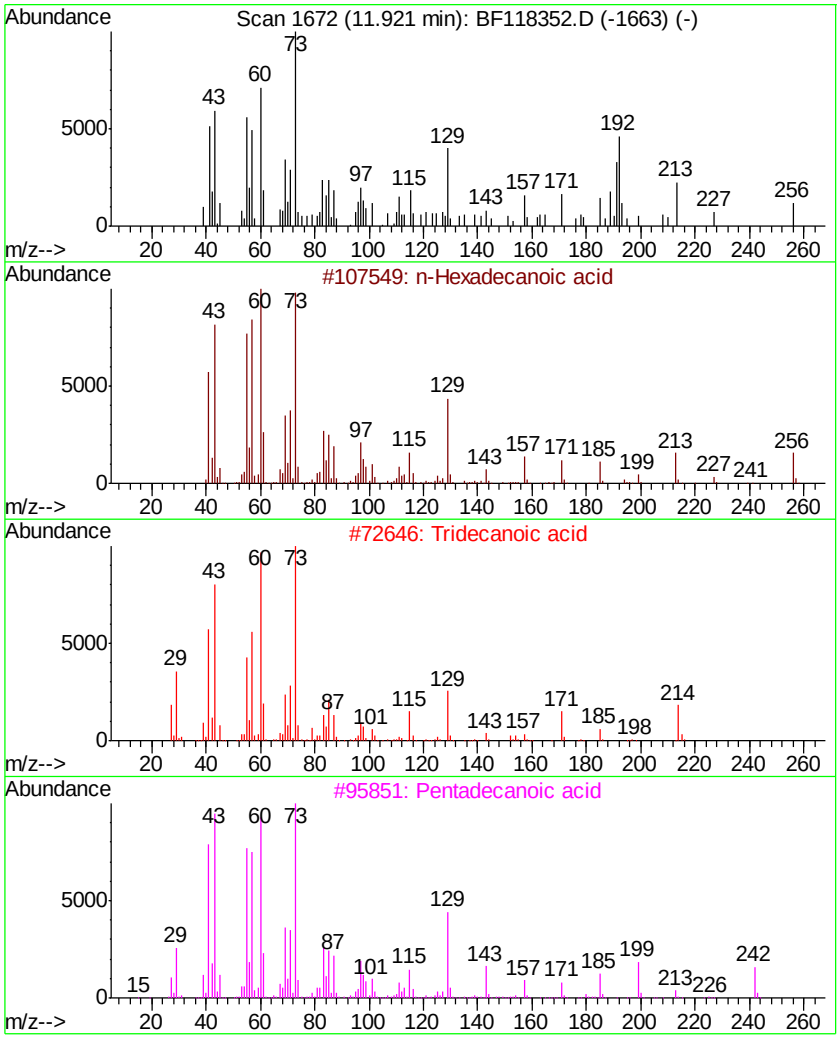
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

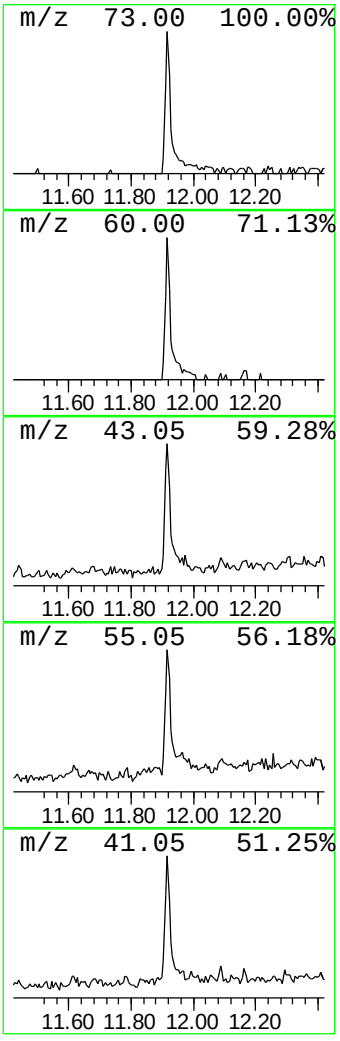
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.45 ng	205868	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

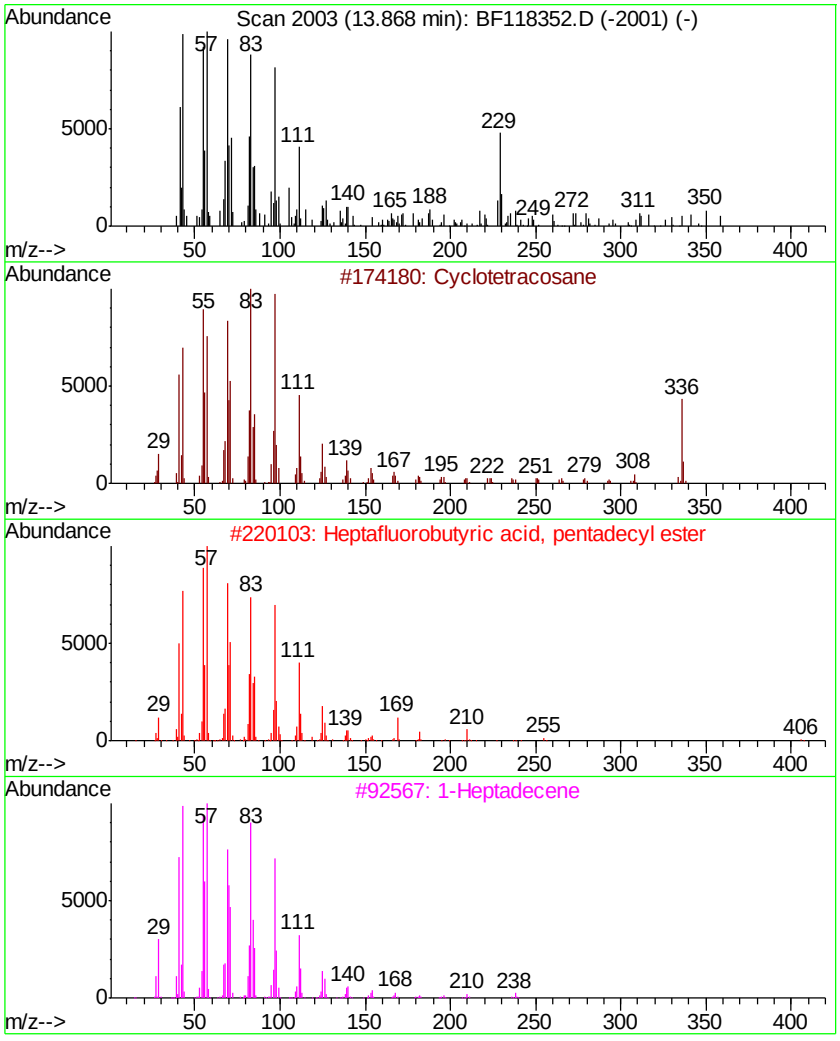
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

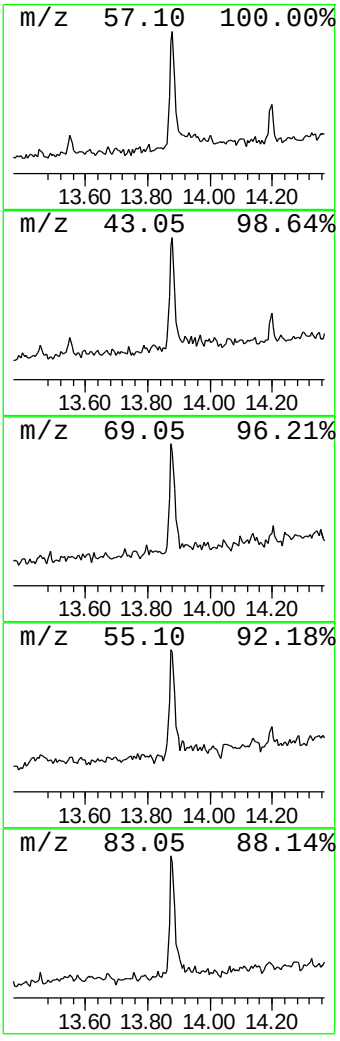
****

Peak Number 5 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.11 ng	244418	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Heptadecene	238	C17H34	006765-39-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122719\
Data File : BF118352.D
Acq On : 27 Dec 2019 21:59
Operator : JU
Sample : K6431-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	5.4	ng	216833	1	6.85	804218	20.0
unknown6.62	6.62	33.9	ng	1363930	1	6.85	804218	20.0
n-Hexadecanoic acid	11.92	4.5	ng	205868	4	11.40	925509	20.0
Cyclotetracosane	13.87	4.1	ng	244418	5	14.05	1189220	20.0